PB88-239041

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(U.S.) Environmental Protection Agency
Research Triangle Park, NC

Jul 88

U.S. Department of Commerce
National Technical Information Service
NTIS

PB88-239041

EPA/600/D-88/163
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TECHNICAL REPORT DATA
(Please read Instructions on the reverse before completing)

1. REPORT NO.	2.	3. RECIPIENT'S ACCESSION NO.
EPA/600/D-88/163		PB88-239041

4. TITLE AND SUBTITLE	5. REPORT DATE
Comparison of EPA Test House Data with Predictions of an Indoor Air Quality Model	July 1988
	6. PERFORMING ORGANIZATION CODE
7. AUTHOR(S)	8. PERFORMING ORGANIZATION REPORT NO.
Leslie E. Sparks, Merrill D. Jackson, and Bruce A. Tichenor	
9. PERFORMING ORGANIZATION NAME AND ADDRESS	10. PROGRAM ELEMENT NO.
See Block 12.	11. CONTRACT/GRANT NO. NA (Inhouse)
12. SPONSORING AGENCY NAME AND ADDRESS	13. TYPE OF REPORT AND PERIOD COVERED
EPA, Office of Research and Development Air and Energy Engineering Research Laboratory Research Triangle Park, NC 27711	Published paper; 6-12/87 14. SPONSORING AGENCY CODE EPA/600/13

15. SUPPLEMENTARY NOTES Principal author Sparks' mail drop is 54; his phone number is 919/541-2458.

16. ABSTRACT An easy-to-use indoor air quality (IAQ) model is described. It is multi-compartmented and based on a well-mixed mixing model. Sources and sinks are allowed in each compartment. A menu-driven fill-in-the-form user interface controls program flow and is used to obtain data from the user. On-screen graphical output is provided. The model estimates the effects of heating, ventilation, and air conditioning (HVAC), air cleaning, room-to-room air movement, and natural ventilation on pollutant concentrations. Experiments conducted in the EPA test house using moth crystal cakes for model verification are described. The agreement between small chamber emission factors, model predictions, and test house data is very good. Predicted weight loss of the moth crystal cakes was within 5% of the measured weight loss. Predicted room concentrations of p-dichlorobenzene are within 20% of the measured values. Future directions for model development and experimental studies are discussed.

17. KEY WORDS AND DOCUMENT ANALYSIS

a. DESCRIPTORS	b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group
Pollution Mathematical Models Mothproofing Insecticides Ventilation Test Facilities Atmosphere Contamination Control	Pollution Control Stationary Sources Indoor Air Quality Moth Crystals Para-dichlorobenzene	13B 14B 12A 06K 13H 06F 13A

18. DISTRIBUTION STATEMENT	19. SECURITY CLASS (This Report)	21. NO. OF PAGES
Release to Public	Unclassified	20
	20. SECURITY CLASS (This page) Unclassified	22. PRICE A03 12.95

EPA Form 2220-1 (9-73)

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Abstract
An easy to use indoor air quality (IAQ) model is described. It is a multi-compartment model based on a well-mixed mixing model. Sources and sinks are allowed in each compartment. A menu-driven fill-in-the form user interface is used to control program flow and obtain data from the user. On-screen graphical output is provided.

The model estimates the effects of heating, ventilating, and air-conditioning (HVAC), air cleaning, room to room air movement, and natural ventilation on pollutant concentrations. Experiments conducted in the EPA test house using moth crystal cakes for model verification are described. The agreement between small chamber emission factors, model predictions, and test house data is very good. Predicted weight loss of the moth crystal cakes was within 5 percent of the measured weight loss. Predicted room concentrations of p-dichlorobenzene are within 20 percent of the measured values. Future directions for model development and experimental studies are discussed.

Introduction

Indoor air quality is determined by the interactions of sources, sinks, and air movement between rooms and between the building and the outdoors. Sources may be located in rooms, in the HVAC system, or outside the building. Sinks may be located in the HVAC system or in rooms, and may also act as sources when the pollutant concentrations drop below a given value.

Air movement in a building consists of:

1. Natural air movement between rooms.
2. Air movement driven by a forced air system (HVAC).
3. Air movement between the building and the outside.

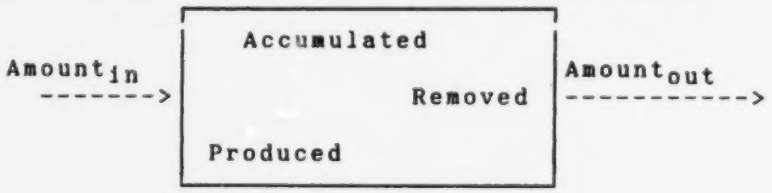

Figure 1. Single room mass flows.

The pollutant concentration in a room is calculated by a mass balance of the various pollutant flows. For the single room shown in Figure 1:

Amount in - Amount out + Amount produced - Amount removed = Amount accumulated

The analysis can be extended to multiple rooms by writing a system of equations for each room. The amount of air entering a room from all sources (the HVAC, outdoors, and other rooms) must equal the amount of air leaving the room.

The type of mixing between the pollutant and the room air must be specified before the mass balance equations can be used in a model. Because mixing is a complex phenomenon, the exact mixing cannot be specified, simplifying assumptions must be made. Plug flow mixing and well-mixed mixing are two common mixing possibilities.

In the plug flow mixing model, the pollutant concentration varies from point to point along the airflow path. In the well-mixed model, the pollutant concentration is the same for every point in the room.

The current model uses the well-mixed model. This model was selected because data from the EPA test house showed that pollutant concentrations within a room do not vary significantly with position in the room (Jackson et al. 1987).

Once the mixing is defined, the various mass balances discussed above can be used to write a set of linear differential equations. These equations can be solved using many techniques. The simplest technique is to approximate the differential equations by difference equations and then solve the difference equations by stepping through time. The equation for two rooms becomes:

Room 1

$$C_1 = t/V_1(C_2Q_{2-1} + C_0Q_{0-1} - C_1Q_{1-2} - C_1Q_{1-0} + S_1 - R_1)$$

Room 2

$$C_2 = t/V_2(C_1Q_{1-2} + C_0Q_{0-2} - C_2Q_{2-1} - C_2Q_{2-0} + S_2 - R_2)$$

where C_1 and C_2 are the concentrations in rooms 1 and 2, t is time, V_1 and V_2 are the volumes of rooms 1 and 2, Q_{1-2} is volumetric flow rate from room 1 to room 2, Q_{0-1} and Q_{0-2} are the volumetric flow rates from the outside into rooms 1 and 2, Q_{2-1} is the volumetric flow rate from room 2 to room 1, Q_{1-0} and Q_{2-0} are the volumetric flow rates from rooms 1 and 2 to the outdoors, S_1 and S_2 are the source terms for rooms 1 and 2, and R_1 and R_2 are the removal (sink) terms for rooms 1 and 2. The initial conditions are: at t=0, $C_1=C_{i1}$ and $C_2=C_{i2}$ where C_i is the initial concentration.

The concentration at any time, t, can be found by stepping through the solution a small time step at a time.

In general the difference equations will give a stable and accurate solution to the equations if the time step is small enough. When the room volumes are of about the same size, large time steps can be used with little difficulty (unless the source and sink terms exhibit short term time behavior). However, when the room volumes differ by orders of magnitude, as is possible when an HVAC system is included in the model, small time steps (5 seconds or less) are needed to avoid numerical instabilities.

The User Interface

A key design goal of the indoor air model was ease of use. A model is of little worth if it is hard to use. Therefore, a menu-driven "fill in the form" data-input user interface was selected. This interface is easy to use and is self prompting. The user interface allows the user to change the input parameters quickly and easily and allows rapid analysis of several conditions.

A master menu controls the operation of the program. The master menu is shown in Figure 2.

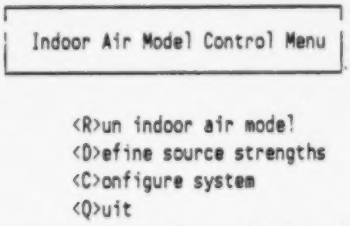

Figure 2. Master menu for AEERL indoor air model.

The model can be configured for various personal computers. It can run on a computer with a monochrome adapter, a color graphics adapter (CGA), or an enhanced graphics adapter (EGA). When the model is run with a monochrome adapter, all graphics are disabled.

Data entry is handled with a "fill in the form" interface. An example form used in the model is shown in Figure 3.

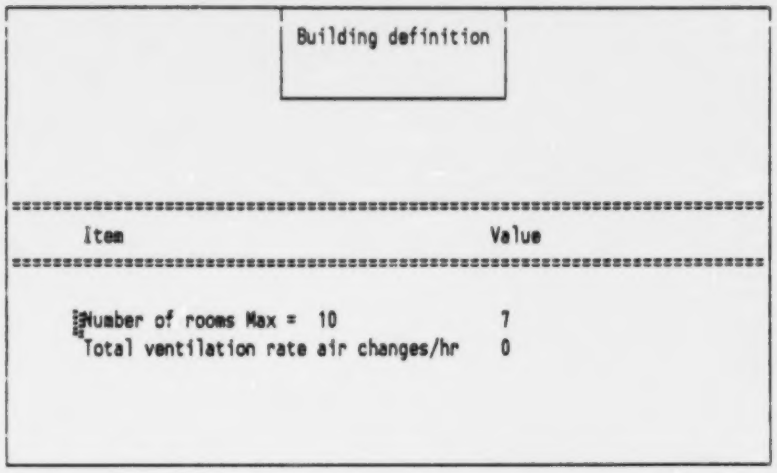

Figure 3. Example form used in model.

The form shown in the example is used to enter the number of rooms in the building and the total ventilation rate.

The most complicated form used in the model is the room definition form, which is used to obtain data on individual rooms in the building. An example of this form is shown in Figure 4.

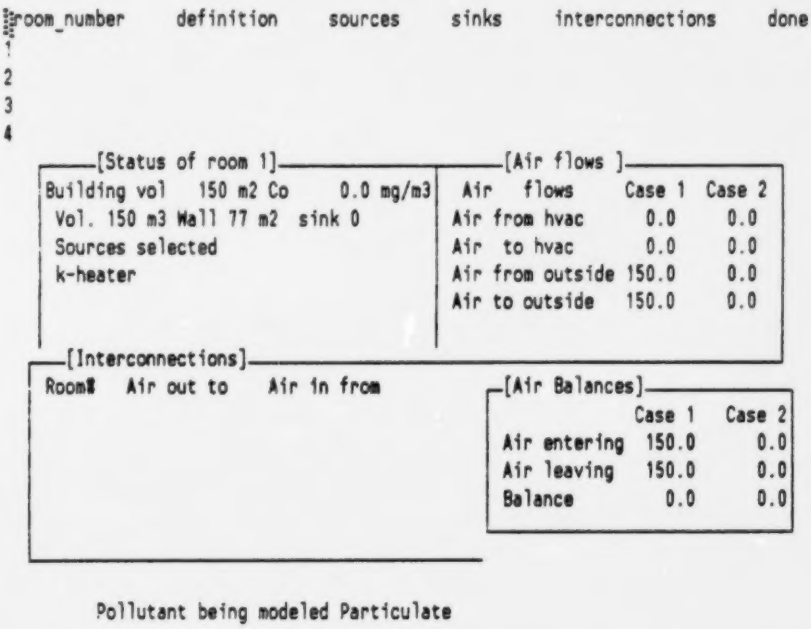

Figure 4. Room definition screen.

This figure shows the overall room definition screen. The options available from this screen are:

- Select room number
- Define room size and initial concentration (definition)
- Define sources
- Define sinks
- Define interconnections with outside, HVAC, and other rooms.

The various options are selected by moving the highlight bar across the top of the screen using the left and right arrow keys.

The results of the model calculations are displayed as plots of concentration versus time for the various rooms. The plots require that a graphics adapter and suitable monitor be installed on the computer.

Source Terms

A wide range of source terms are available in the model including random on/off sources (cigarettes), sources that are on for a specified period of time (heaters), steady-state sources (moth crystals), and sources with high initial emission rates followed by low steady-state (floor wax). The IAQ model accommodates all these possibilities in an idealized fashion. Each of the sources in the model is discussed below.

Cigarette Smoking

Cigarette smoking is modeled as a random event with from 1 to n cigarettes smoked per hour. The cigarette is turned on at some random time during the hour. A second cigarette is not allowed on until the first cigarette is smoked. Multiple smokers are accommodated in the model; however, all smokers smoke at the same time.

Unvented Kerosene and Gas Heaters

Unvented kerosene and gas heaters are common sources of indoor air pollution. These heaters are modeled as steady-state on/off heaters. The on- and off- times are part of the data input to the program. Up to three on/off cycles per day are allowed.

Moth Crystal Cakes

Moth crystal cakes can be an important source of volatile organic compound (VOC) emissions indoors. Moth crystal cakes are long-term steady-state sources. The emissions from moth crystals are a function of the temperature and the surface area of the cakes.

Floor Wax

Floor wax is an example of a "wet" source of VOC emissions. Wet sources have an initial very high emission factor followed by a low-level, steady-state emission factor.

The emission factor for floor wax is based on work conducted by EPA and is shown in Figure 5 (Tichenor et al. 1987). The curve in Figure 5 can be approximated by equations of the form emission = $(a_1)\exp(-a_2 t)$ where a_1 and a_2 are constants.

Other

The "other" source is provided as a user defined steady state source. The source cannot be turned off.

Sinks

It is generally recognized that walls and furnishings can serve as collectors (sinks) of indoor air pollutants. Unfortunately, the data on sinks are limited. The model allows investigation of the behavior of sinks by providing a single sink that is a function of the surface area of the walls in the room. This sink is a pure sink; i.e., pollutants trapped by the sink are not re-emitted.

Small chamber and test house studies are planned to provide fundamental data on sink behavior. The results of these studies will be incorporated into the model as soon as they are available.

The Air-Handling System

The airflows generated by an air-handling system are generally larger than natural airflows. Thus, when an HVAC system is on, the building's airflows are dominated by the HVAC system. Airflow patterns in a building with the air-handling system on may be significantly different from airflow patterns in the same building with the air-handling system off. For example, many houses have a single return vent for the air-handling system. When the air-handling system is on, airflow is dominated by the flow to the return vent. When the air-handling system is off, airflow is less directed.

The on/off behavior of the air-handling system is modeled by allowing two different airflow patterns to exist in the building. One pattern is active when the air-handling system is on and the other when the air-handling system is off. The model switches between these two patterns depending on the state of the air-handling system. The state of the air-handling system (on or off) is determined by a random number generator designed to ensure that the air-handling system is on for a specified fraction of each hour. The air-handling system may switch from on to off and back several times in an hour. This random switching appears to provide a qualitative description of actual air-handling system behavior. Experiments are planned to determine how well the model fits actual air handler behavior.

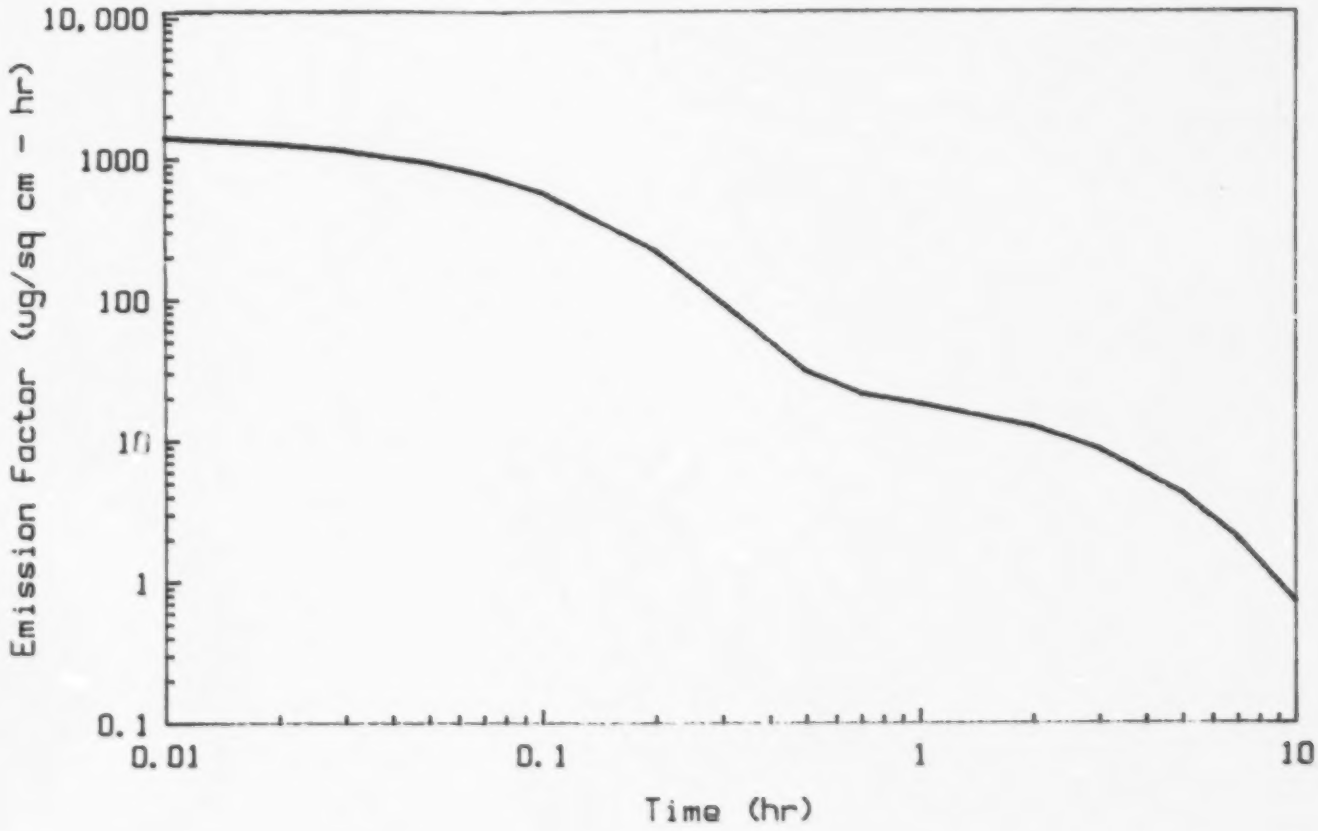

Figure 5. Floor wax emission factors (Tichenor et al., 1987).

Air Movement Data Needed for the Model

Although the model could have been written to calculate the interroom airflows, it was decided to require the user to enter them. Calculation of the interroom airflow requires knowledge of the temperature and pressure gradients between rooms. This information is generally not available and would thus have to be estimated. We believe that it is better to estimate the airflows directly instead of calculating them from estimates of temperature and pressure gradients.

We also believe that requiring the user to enter the interroom airflows gives the user a better understanding of the interactions between airflows from different rooms.

Limited sensitivity analysis of the model shows that interroom airflows do not have to be estimated with high precision to produce good model results. Generally there is more than enough air movement in a building to provide adequate room-to-room pollutant mixing.

Comparison to National Bureau of Standards Model

The model predictions were compared to the predictions from the National Bureau of Standards (NBS) model (Axley 1987) to ensure that the numeric techniques used in the model were satisfactory. The agreement between the two models was excellent. This is not surprising, since both models are mass balance models. An example of the agreement between the two models is shown in Figure 6.

Comparison of Data from EPA Test House with Model Predictions

The final proof of a model is how well it fits experimental data. This section provides a comparison of the model predictions with data from the EPA test house. The section also demonstrates how small chamber emission factors can be used in the model to predict IAQ pollutant concentrations.

Chamber studies to determine the p-dichlorobenzene emission factor from moth crystals were conducted before the test house experiment. The small chambers have a volume of 166 L (liters). The experimental techniques are described by Nelms et al.(1987). The emission factor developed by Nelms et al. for the conditions in the test house experiment is 1.4 mg/cm^2-hr.

EPA has rented a three-bedroom ranch style house to serve as a test house for IAQ studies. The floor plan of the test house is shown in Figure 7.

Blower door and SF_6 tracer experiments were conducted to determine the air infiltration rates for the test house. These experiments established an infiltration rate of 0.35 air changes per hour (ACH) for the weather conditions of the moth crystal experiment.

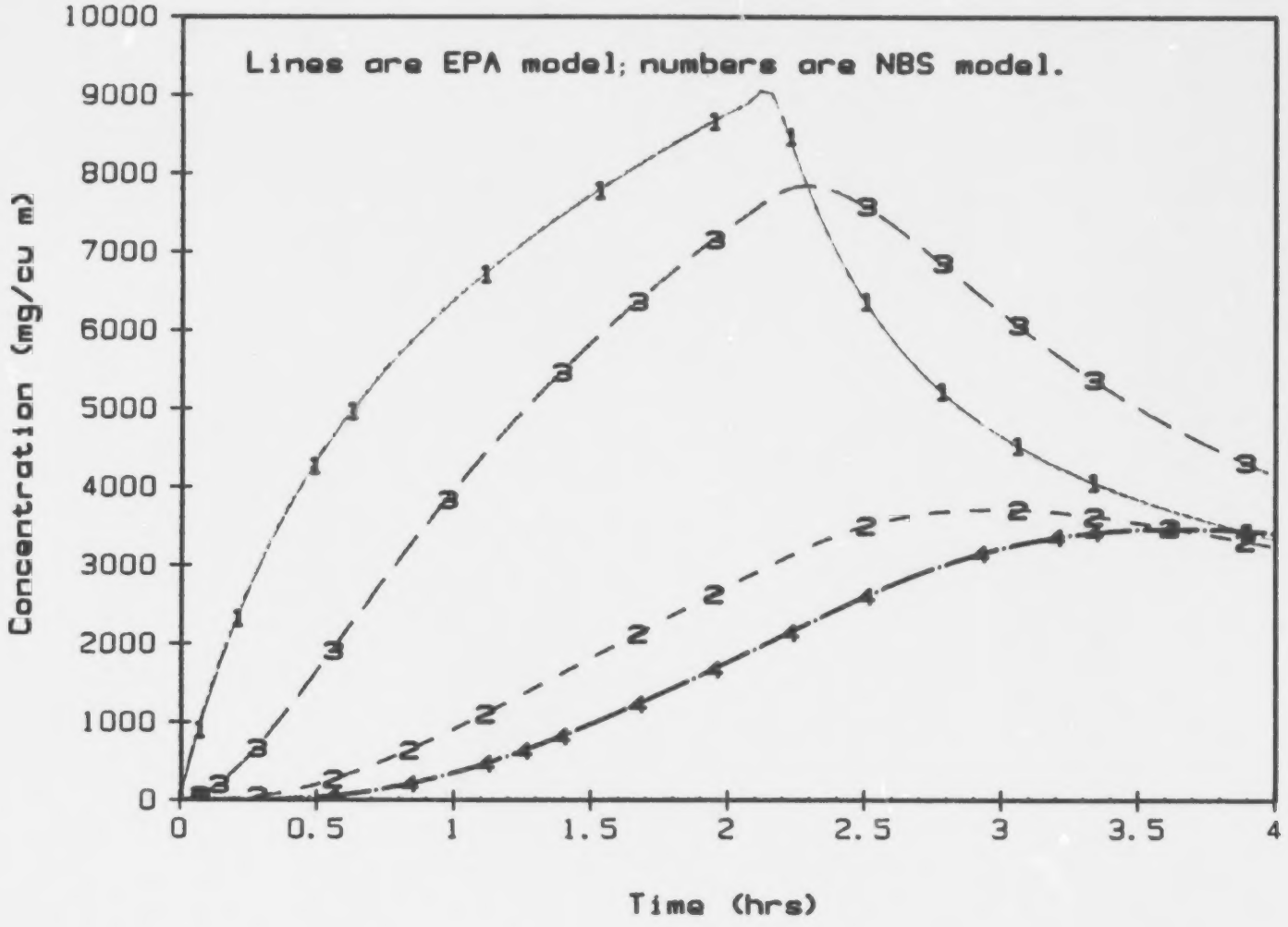

Figure 6. Comparison of EPA model predictions with NBS model predictions, Axley (1987).

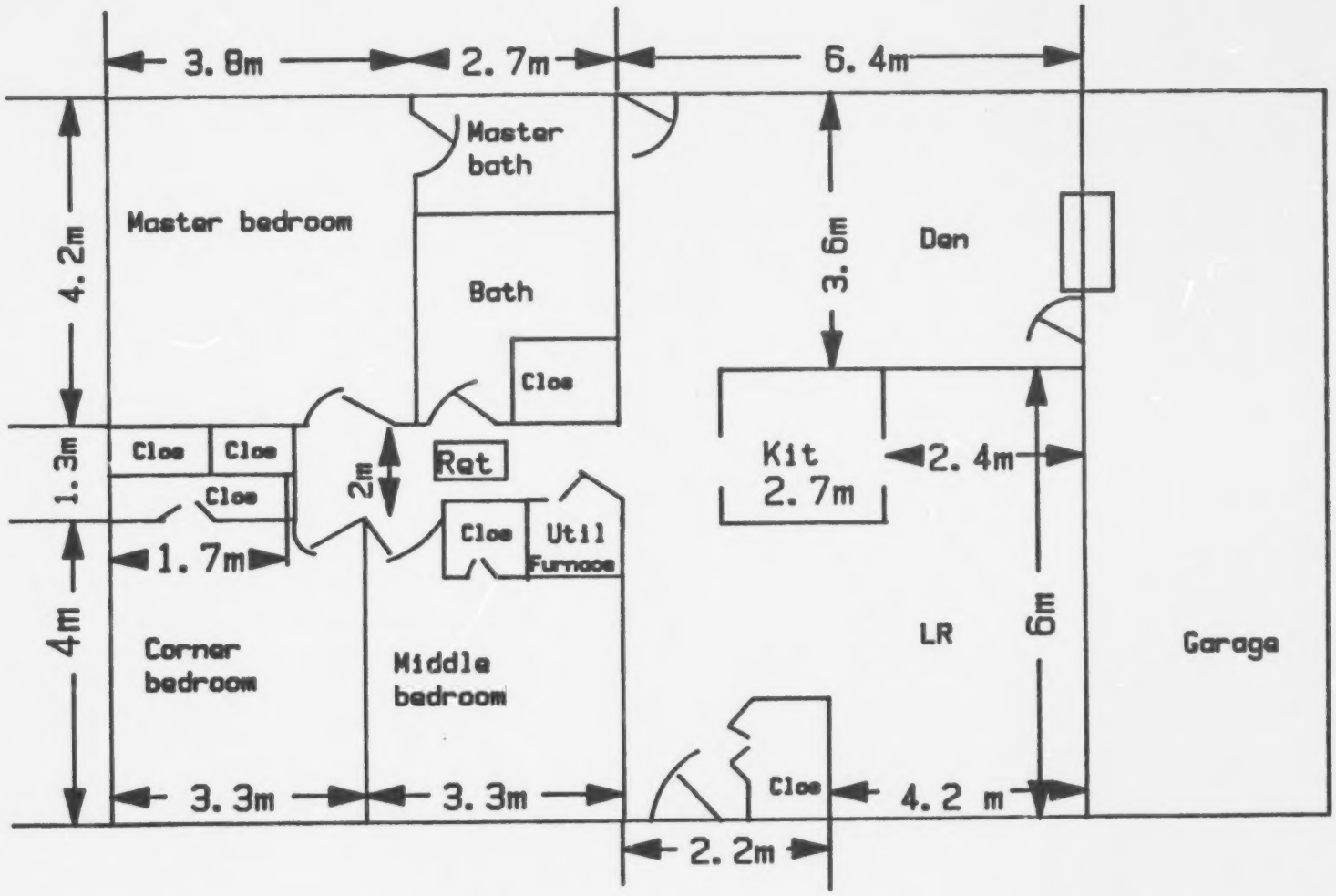

Figure 7. EPA IAQ test house.

CO_2 was injected into the corner bedroom at a constant rate during the moth crystal experiments. The CO_2 concentrations were determined in the closet, the corner and master bedrooms, and the den. The CO_2 data were analyzed to determine if there were major changes in the infiltration of outside air into the house. The CO_2 data were essentially constant for the duration of the experiment. This indicates that for the seven days of the experiment, there were no significant changes in the infiltration of outdoor air.

For the moth crystal experiments, five cakes of moth crystals were placed in the closet in the corner bedroom. The moth crystals were laid on the shelves and had an exposed surface area of 570 cm^2. The air-handling system operated continuously for the entire experiment.

P-dichlorobenzene concentrations were measured in the closet, in the corner bedroom, in the master bedroom, and in the den. The p-dichlorobenzene measurements were made by direct injection into the gas chromatagraph and were made once a day for four days. The first measurement was made three days after the moth crystal cakes were placed in the closet.

The results of the four days of measurements are shown in Table 1.

TABLE 1

Results of p-dichlorobenzene Measurements, mg/m^3				
Day/Room	Closet	Corner bedroom	Master bedroom	Den
1	107	4.72	3.49	3.84
2	53.6	4.41	3.50	3.30
3	70.9	5.51	4.18	3.80
4	63.0	5.61	4.27	4.02

The differences between day to day measurements in Table 1 are probably normal data scatter. Nothing should be inferred from the apparent trends.

An average p-dichlorobenzene emission factor was calculated by dividing the total weight lost by the moth crystals by the duration of the experiment. The average emission factor was 820 mg/h or (1.44 mg/cm^2-h) which is in excellent agreement with the small chamber emission factor.

P-dichlorobenzene concentrations were measured for seven days after the moth crystals were removed from the closet. The concentrations were still above 0.5 mg/m^3 at the end of the seven days. This suggests that there was a strong sink for p-dichlorobenzene in the test house.

The concentration data in Table 1 and the average emission factor can be used to estimate the sink effect. The analysis is based on treating the house as a single chamber. The mass balance for the entire house at any time, t, gives:

$$dc/dt = E(t) - Qc_t$$

where dc/dt is the change of p-dichlorobenzene concentration in the house as a function of time, Q is the airflow through the house, E(t) is the emission rate (which may be a function of time), and c_t is the concentration in the house at time t. The equation can be rearranged to allow calculation of E(t):

$$E(t) = dc/dt + Qc_t$$

An effective emission rate, $E_e(t)$, was obtained by smoothing the concentration data using a robust regression (Ingels and Pallette 1987) and then calculating dc/dt from the smooth curve. $E_e(t)$ for various times was then calculated. An average effective emission rate was calculated from the $E_e(t)$ curve. The average effective emission rate was 480 mg/hr. This compares with an average emission rate of 820 mg/hr based on the weight lost by the moth crystals during the experiment. The difference between the emission rate calculated from the weight loss and the effective emission rate calculated from the house concentration data is the sink term. The sink term is 340 mg/hr.

Initial model runs with the sink term and estimates of the room-to-room airflows were in good agreement with the measurements for all rooms except the closet. The closet concentrations were a factor of 13 too high (see Table 4). Also, the den and master bedroom concentrations were too low relative to the corner bedroom concentration. Additional model runs showed that the flow from the closet to the corner bedroom was the key unknown parameter for determining the p-dichlorobenzene concentrations in the house.

Therefore, experiments were conducted to define the airflows in the test house and to estimate the type of mixing. During these experiments, the air-handling system flows were measured. Flow visualization studies to determine the nature of the in-room and room-to-room mixing were conducted with neutral density balloons and with neutral density helium bubbles.

The measured flows of the air-handling system are shown in Table 2.

TABLE 2

Air-Handling System Airflows in Test House

Room	Measured air flow, m^3/hr
Den	679
Middle bedroom	38
Corner bedroom	278
Master bedroom	280

The balloon and bubble experiments showed that, even with the air-handling system on, considerable mixing existed between rooms. These experiments also indicated that there was a substantial airflow into and out of the closet. Finally, the visualization studies indicated that there was flow between the closet and the hallway and between the closet and the master bedroom.

Hot-wire anemometer measurements were made of the airflow velocities through the cracks in the closet door. These measurements showed that the airflow into and out of the closet was between 4 and 9 m^3/hr.

Model calculations were performed with the input data from the experimental studies. The input data for the model run are shown in Table 3. The model calculations were stopped after several hours of simulated time because steady-state was reached.

TABLE 3

Input Data for Moth Crystal Analysis

Source strength, 1.4 mg/cm^2-hr, Nelms et al.(1987).
Air exchange with outside, 0.35 ACH (SF_6 data).
Air exchange between closet and bedroom, 4 m^3/hr.
Air circulation to air-handling system as in Table 2.
All airflow to air-handling system is from hallway.
Air exchange with outside is evenly divided between rooms.
Sink removes 40 percent of material.

The results of this run are shown in Figure 8. The agreement between the model and the measured data is excellent for all rooms.

Several additional runs were made to determine the effects of errors in the input data. Runs were made with low flow from the closet, no sink, a large sink, and errors in estimating the interroom flows. A summary of the model results is presented in Table 4.

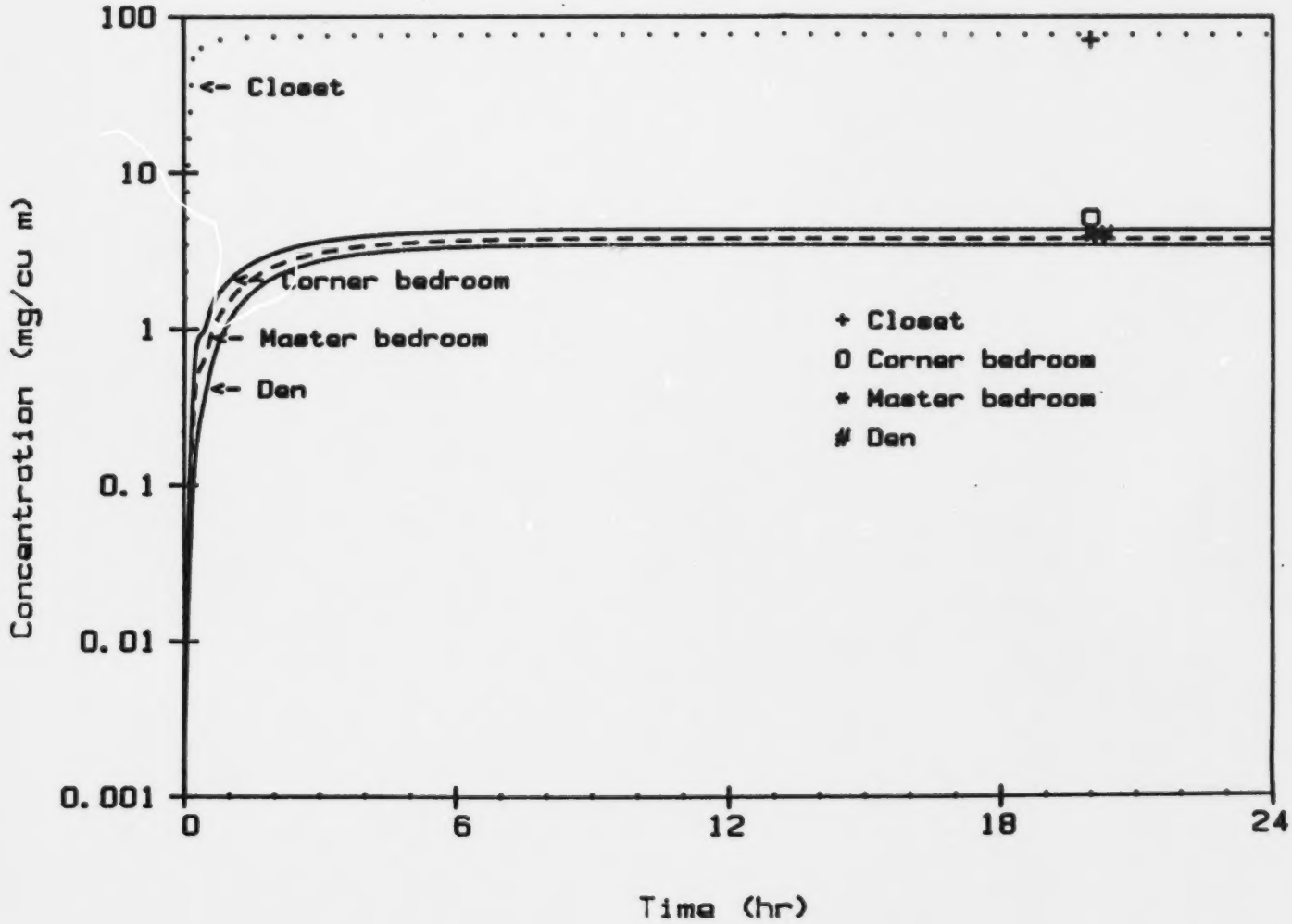

Figure 8. Final IAQ model run for moth crystal data.

TABLE 4

Summary Comparison of Model Predictions and Measured Data
Ratio of predicted to measured concentrations

Case	Closet	Corner Bedroom	Master Bedroom	Den
1	13	0.96	0.85	0.87
2	1.1	0.048	0.025	0.027
3	3	1.8	2.2	2.2
4	0.998	0.89	0.97	0.93

Measured concentration is average of all measurements
Case 1: Low flow from closet and sink (initial run).
Case 2: Low flow from closet and large sink.
Case 3: 4 m^3/hr flow from closet and no sink.
Case 4: Measured flows and sink.

Use of the Model to Analyze Mitigation Strategies

One of the powerful uses of the model is analysis of mitigation strategies. This can be demonstrated by an analysis of options for reducing p-dichlorobenzene concentrations in the house. The options are: (1) reduction of the amount of moth crystals used, (2) reduction of flows from the closet, and (3) a combination of reduced flows and use of moth crystals. The constraints imposed were: p-dichlorobenzene concentrations in the closet must not drop below 25 mg/m^3 and p-dichlorobenzene concentrations in the house must not exceed 0.5 m^3. (Note, the constraints used in this example are arbitrary. The purpose is to demonstrate the use of the model and not to indicate levels necessary for moth control or elimination of effects.)

The model results showed that reducing the moth crystal loading by 80 percent maintained over 25 mg/m^3 in the closet but the concentrations in the rest of the house were greater than 1 mg/m^3. Reducing the flow from the closet met both constraints as did a combination of reduced moth crystal use and reduced flow.

Conclusions

The study described here demonstrates that small chamber data can be used with a model to predict pollutant concentrations in the EPA test house. The study also shows that, when IAQ is dominated by a large point source, knowledge of the source strength and rough estimates of the various airflows are sufficient to predict concentrations within reasonable (± a factor of 2) accuracy for much of the building. The most important airflow is that from the room with the point source to adjacent rooms.

Finally, the moth crystal study showed that, when data are available for most parameters important for the model, the model predictions are in excellent agreement with the measured values.

The model is a powerful tool for evaluating IAQ control options. The ease of use makes it possible to run the model several times to determine effectiveness of control options.

Future Plans

The case study discussed above, while important, is a single study for a relatively simple case. Additional research is necessary to prove the feasibility of using small chamber emission factors and the model to predict IAQ for complicated situations. Additional work on sinks is especially important. Some of the necessary research is planned for the current calendar year (1988). Solvent based floor waxes, aerosol products, and various activity sources are among the sources that will be studied.

Air flow studies are also planned. These studies will allow analysis of the model's handling of the on/off air handler.

Additional work is planned on the model itself. The main thrust of the modeling work will be on increasing the computational speed and on improving the user interface. Several techniques are being investigated. Work will also be conducted to develop a set of default values for room to room flows under a range of situations.

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